CONTENTS

Special Issue: Six Decades of the Hybridization Model – A Tribute to Linus Pauling, 1954 Nobel Prize-winner in Chemistry and 1962 Nobel Peace Prize-winner.

Review: The six decades of the hybrid concept
C. Yang (Suzhou, People's Republic of China) 1
Some new properties of the reduced density operator and derivation of molecular electronic entropy
J.A. Medrano and R.C. Bochicchio (Buenos Aires, Argentina) 33
Analysis of the geometry of the hydroxymethyl radical by the "different hybrids for different spins" natural bond orbital procedure
J.E. Carpenter and F. Weinhold (Madison, WI, U.S.A.) 41
Resonating structures versus molecular orbitals: a problem of electron correlations
P. Fulde (Stuttgart, F.R.G.) 63
Rehybridization in nonplanar conjugated organic molecules: transformation of the π-orbital axis vector (POAV) analysis to the equivalent orbital bent-bond representation
R.C. Haddon (Murray Hill, NJ, U.S.A.) 69
Hybridisation is not arbitrary
D.B. Cook (Sheffield, Gt. Britain) 79
The role of hybridization in perturbative bond theories: the existence of exact strictly localized orbitals in small molecules
P.R. Surján (Budapest, Hungary) 95
Electrostatic interactions and the shape of van der Waals dimers
V. Magnasco, C. Costa and G. Figari (Genova, Italy) 105
Hybridization and valence angle dependence of *geminal* NMR coupling constants
M. Klessinger and P. Bolte (Münster, F.R.G.) 119
Is hybridization just an artefact or does it reflect some physical reality?
A. Julg (Marseille, France) 125
Bent bonds, hybrid orbitals and photoelectron spectroscopy
R.P. Messmer (Philadelphia, PA, U.S.A.) 137
The electronic and geometric structures of the early transition metal cations MCH^+, MCH_2^+ and MCH_3^+
A.E. Alvardo-Swaisgood and J.F. Harrison (East Lansing, MI, U.S.A.) 155
Pauling–Wheland resonance theory of benzenoid hydrocarbons
D.J. Klein and W.A. Seitz (Galveston, TX, U.S.A.) 167
Hybridization and the interaction of diabatic states
G.A. Gallup (Lincoln, NE, U.S.A.) 183
Qualitative valence bond theory: speculations concerning the origin of some bond-length variations
R.D. Harcourt (Parkville, Vic., Australia) 193
An interpretation of chemical bonding in a molecular orbital wavefunction
A. Chung-Phillips (Oxford, OH, U.S.A.) 211
Resonance and reactivity
G.G. Hall (Kyoto, Japan) 233
Localized molecular orbitals of simple metal–olefin complexes
D.S. Marynick and C.M. Kirkpatrick (Arlington, TX, U.S.A.) 245
The localized orbital approach to molecular structure
G. Leroy and D. Peeters (Louvain-la-Neuve, Belgium) 257

Small scale variational scheme incorporating local orbitals with fully flexible hybridization: a local orbital reconstruction of Walsh's rules
C. Trindle (Charlottesville, VA, U.S.A.) 273
The electronic structure of methane and its derivatives: apparent versus effective symmetry control of sigma bonding
N.D. Epiotis (Seattle, WA, U.S.A.) 289
Direct calculation of delocalization and resonance energies using truncated LMOs
C. Edmiston (Laramie, WY, U.S.A.) 331
Bonding and electronic structure in diatomic ThO: quasirelativistic effective core potential calculations
C.M. Marian, U. Wahlgren (Stockholm, Sweden), O. Gropen (Tromsø, Norway) and P. Pyykkö (Helsinki, Finland) 339
Bond bending and hybridization
K.B. Wiberg and M.A. Murcko (New Haven, CT, U.S.A.) 355
Atomic orbitals in the ab initio analysis of imidazole H-bonding
F. Zuccarello, G. Buemi (Catania, Italy) and G. Del Re (Napoli, Italy) 367
Determination of atomic hybridization in molecular orbital theory: a valency method
M.S. Gopinathan (Madras, India) 379
Charges and bond orders in covalent xenon compounds using the structure–resonance paradigm
W.C. Herndon (El Paso, TX, U.S.A.) 389
Orthogonal and non-orthogonal hybrids
W. Kutzelnigg (Bochum, F.R.G.) 403
The ab initio spin-coupled description of methane: hybridization without preconceptions
F. Penotti, J. Gerratt (Bristol, Gt. Britain), D.L. Cooper (Liverpool, Gt. Britain) and M. Raimondi (Milano, Italy) 421
Valence bond calculations of the degree of covalency in a C–X bond: application to CH_4 and CH_3Li
P.C. Hiberty (Orsay, France) and D.L. Cooper (Liverpool, Gt. Britain) 437
Protonation and rehybridization: a combined ab initio and semiempirical study
Z.B. Maksić, M. Eckert-Maksić (Zagreb, Yugoslavia), P.N. Skancke and A. Skancke (Tromsø, Norway) 447
Hybridization in valence bond theory: the water molecule
R. McWeeny (Pisa, Italy) and F.E. Jorge (Vitóroa, Brazil) 459
Neutral eigenstates of extended systems: resonance of neutral VB structures or perturbation of (Neel states) spin waves?
P. Blaise, J.P. Malrieu. D. Maynau and B. Oujia (Toulouse, France) 469
On the general theoretical foundations of methods for optimum hybrids
G. Del Re (Napoli, Italy) 487
Ab initio calculations of the Raman intensities of fundamental vibrations of polyatomic molecules using the improved virtual orbital technique
P. Raeymaekers, H. Figeys and P. Geerlings (Brussels, Belgium) 509
Strain in three-membered rings containing silicon: the inability of silicon to form flexible hybrid orbitals
D. Cremer, J. Gauss and E. Cremer (Köln, F.R.G.) 531

Short communication
Theoretical studies of triquinacene and diademane
J.M. Schulman, M.A. Miller and R.L. Disch (Flushing, NY, U.S.A.) 563

Author index 569

Subject index 570